

**[o.m10.o3] Modulations and Disorder in a Perydrotriphenylene Inclusion Compound.**Th. Weber, H.B. Bürgi, *Univ. of Berne, Freiestr. 3, CH-3012 Bern.*

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The host structure of perhydrotriphenylene (PHTP) inclusion compounds is built from stacks of triangular shaped PHTP molecules forming a pseudo-hexagonal arrangement of tunnels of infinite length which host a lattice of guest molecules. Because host-host, guest-guest and host-guest interactions, i.e. interactions within and between sublattices, are mainly due to weak dispersion forces, the molecular arrangement is very sensitive to the properties of local intermolecular contacts and shows a richness of disorder phenomena and modulation with long-range order. An investigation was undertaken of the resulting diffuse and satellite scattering of the inclusion compound with 1-(4-nitrophenyl)piperazine (NPP) to study supramolecular building principles in crystals where no strong intermolecular interactions are present.

Analysis of the Bragg reflexions shows that every PHTP site is occupied with the same probability by either a (+) or a (-)-PHTP molecule. The lattice of NPP molecules is commensurate with that of the host molecules along the tunnel axis ( $c_{\text{guest}} : c_{\text{host}} = 5 : 1$ ). However, the relative positions of the chains of guest molecules in neighbouring channels exhibit positional disorder along the tunnel axis in such a way that the average guest-translation matches that of the host [1].

Diffuse and satellite scattering phenomena may be divided into two categories: 1) strong diffuse intensities in the Bragg layers perpendicular to the tunnel axis  $c^*$  and 2) diffuse intensities and satellites in the layers perpendicular to  $c^*$  at  $l = 0.2, 0.4, 0.6$ , etc. The strong diffuse intensities in the Bragg layers are due to the racemic disorder of the host. Alternation of stacks of (+) and (-)-PHTP molecules in the lateral directions is preferred, but not perfect; neighboring host molecules along  $c$  are preferentially homochiral. A weaker pattern of streak-like scattering within the Bragg layers indicates displacive disorder of PHTP molecules with a strong correlation along the  $a$ -axis and a weaker correlation along  $b$ . The similarity of these features at room temperature and 120 K suggests that they must be due to static disorder. The layers perpendicular to  $c^*$  at  $l = 0.2, 0.4, 0.6$ , etc. contain diffuse intensities and satellites with an incommensurate component parallel to  $a$ . The former is due mainly to the positional disorder of the chains of guest molecules in the lateral directions parallel to  $c$ , whereas the latter is probably due to mutual modulations of host and guest lattices.

Finally, it has been found that, although the Bragg intensities and the positions of the satellites show orthorhombic symmetry throughout the crystal, the symmetry of the satellite intensities is different at the centre and at the tip of the needle-like crystals: orthorhombic at the crystal centre, but monoclinic at the crystal tip. A detailed investigation of the satellite intensities is in progress.

[1] O. König, H.B. Bürgi, Th. Armbruster, J. Hulliger & Th. Weber, *J. Am. Chem. Soc.* 1997, **119**, 10632–10640.

**[o.m10.o4] Diffuse X-ray Scattering and Strain Effects in Disordered Crystals.**T.R. Welberry, *Research School of Chemistry, Australian National University, Canberra ACT 0200, Australia.*

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In numerous recent studies we have observed diffuse X-ray scattering from a wide variety of materials. Although these studies have shown the great variety of diffuse scattering patterns that can exist in different materials, some common features have emerged. One particularly distinctive feature that has been observed in materials as diverse as cubic stabilized zirconia, the aluminosilicate ceramic mullite, the didecyl-benzene/urea inclusion compound and the pure molecular crystal 1,3-dibromo-2,5-diethyl-4,6-dimethyl-benzene, is a diffuse 'ring' or 'doughnut' shaped region of scattering.

In metal alloys such features have been attributed to spinodal decomposition<sup>1</sup>, but more recently Butler & Hanley<sup>2</sup> have shown that such features in the diffraction pattern of sol-gel systems can arise from competition between a short-range attractive and a long long-range repulsive potential. In these systems the short-range attractive forces tend to cause aggregation of particles while the long-range repulsion acts to keep them apart and this results in the formation of space-filling networks. A characteristic diffuse ring is observed in the diffraction pattern which moves toward lower wavevectors as the simulation evolves. However, unlike a pure Lennard-Jones system, which when given enough time will completely phase separate, the diffuse ring attains a stable radius once a network has formed.

In the present paper we discuss how these basic concepts can be carried over to provide insight into the mechanisms governing disorder in the different crystalline materials mentioned above.

[1] Cahn J.W. Spinodal Decomposition, *Trans. Metallurg. Soc. Amer.*, 1967, 168-180.

[2] Butler, B. D.; Hanley, H. J. M. Aggregation in quenched systems interacting through a short-range attractive, long-range repulsive potential. *J. Sol-Gel Sci. Technol.* (1999), 15(2), 161-166.